Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 27.5

Global applicability domain: Inside

Local applicability domain index: 4.69e-01

Confidence level: 6.97e-01

Nearest Neighbors from the Training Set

Image not found
Isophorone
Measured: 2.00
Predicted: 3.19

Image not found
N,N-Diethylaniline
Measured: 102
Predicted: 12.8

Image not found
Benzothiazole
Measured: 7.59
Predicted: 6.05

Image not found
Isoamyl ether
Measured: 170
Predicted: 137

Image not found
5-Ethylidene-2-norbornene
Measured: 110
Predicted: 134